Multiphysics Time Integration and Long Time Integration Error

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Predictive computer simulation of multiphysics systems is one of the Laboratory's core missions. This endeavor is at the heart of such DOE programs as the Advanced Simulation and Computing (ASC) program and the Scientific Discovery through Advanced Computing (SciDAC) program. There are many factors that affect the accuracy of a simulation, including proper physics models, accurate spatial discretization, and adequate spatial grid resolution. Perhaps the least appreciated, understood, and studied factor is the issue of multiphysics time integration methods and long time integration error.

Modern multiphysics time integration methods are comprised of basic time integration methods, and nonlinear and linear solver techniques that can be abstracted and generally applied to accurately, robustly and efficiently solve multiphysics systems. These systems are characterized by a myriad of complex interacting physical mechanisms. These mechanisms often nearly balance to evolve a solution on a dynamical time scale that is long relative to the component time scales. Solution methods for such systems require the use of significant coupling in the nonlinear and linear solution techniques and a significant implicit character to the time integration methods.

The number of time steps required for a multiphysics computer simulation is typically proportional to the ratio of the slowest time scale to one of the faster time scales. Because of this ratio, multiphysics simulations often require many (10^6) time steps. The resulting accuracy after a large number of time steps depends more on a temporal integration schemes ability to track the solution than on the size of the error on a single time step. A temporal integration scheme that drifts away from the solution may end up with a global error that is very large even if it has a small error per time step.

This solution drift error is particularly dangerous because the solution is qualitatively correct and thus there are no obvious symptoms that the error even exists. Because this error currently goes unmeasured in large-scale multiphysics simulations, we must develop a deeper understanding of this weak link in predictive simulation to further quantify this uncertainty.

Within the overall field, we have been working on developing new solution algorithms which are second-order accurate in time, using numerical analysis to understand errors in existing first-order in time methods, and gaining a deeper understanding of how the time integration errors may accumulate within a multiphysics computer simulation. In algorithm development we have focused on Jacobian-Free Newton-Krylov methods with physics-based preconditioners [1] along with second-order in time operator splitting methods [2, 3]. We have concentrated on using modified equation analysis [4] and asymptotic analysis as numerical analysis tools for studying the errors and behaviors of splitting methods.

All of our multiphysics problems of interest have fluid dynamics as the core of the problem, with additional physics contributing to the overall problem. In addition to working with prototype systems, we have been applying our research to multiphysics systems such as radiation hydrodynamics, extended magnetohydrodynamics [5], multiphase flow hurricane systems [6], solidifying flows [7], and nuclear power reactor thermal hydraulics [8].

As a simple example of accumulation of time integration error consider Fig. 1, which displays a solution at two different times (t = 5 and 10) for a one dimensional (1-D) reaction diffusion problem. This is a thermal wave moving left to right in time. The exact solution is EX, BE is a first-order in time solution, and CN is a second-order in time solution. For a given time step we see the first-order method drifting in time from the EX solution, while the second-order in time method tracks the EX solution. Figure 2 shows that even when the two methods have the same local truncation error (LTE) per time step (x-axis), and we integrate to the same time (t = 15), the global error (y-axis) is different. The BE methods drifts from the solution at a faster rate than the CN method and this gap increases as we increase the allowable LTE per time step. This is directly related to our premise that these two different LTE's integrate differently in time since in BE the truncation error is dissipative and in CN the truncation error is dispersive.

As a second example we look at nonequilibrium radiation diffusion. In the asymptotic limit, where the coupling between radiation and material is tight, the two fields should have the same temperature (equilibrium). We have used asymptotic analysis to show that a "standard" split/linearized method for this problem does not enforce this asymptotic balance. In the problem shown in Figs. 3 and 4, a radiation front is moving from left to right heating the material. Solutions are plotted for t = 0.1 and 0.5. There is no physical mechanism for the material temperature, Tm, to be hotter than the radiation temperature, Tr. As shown in Fig. 3, the results coming from an unsplit (implicitly balanced) method show a physically credible solution with the temperatures close, but Tr > Tm. The result in Fig. 4, coming from a split/linearized method, was predicted by our analysis and is not physically correct since Tm > Tr. This analysis has helped to explain a "frequently observed" inaccuracy in such simulations.

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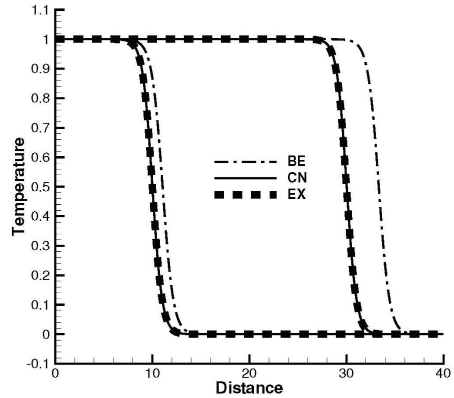

Fig. 1.
Various solutions of the reaction diffusion problem at t = 5 and 10.

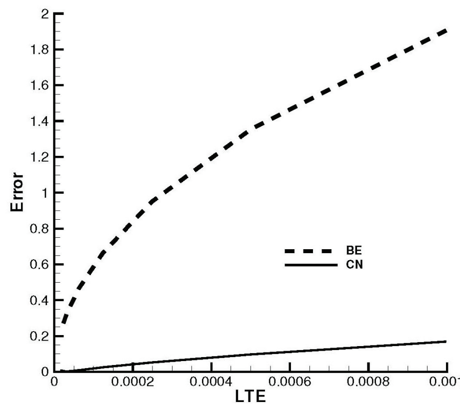

Fig. 2.
Global solution error as a function of LTE per time step.

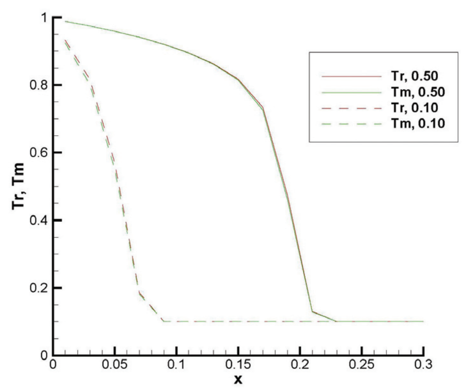

Fig. 3.
Implicitly balanced solution.

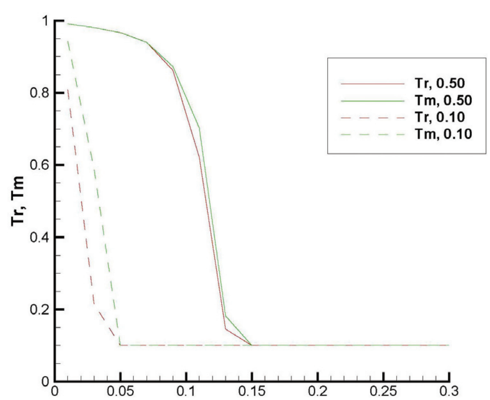

Fig. 4.
Split/linearized solution.

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